

Monte Carlo study of the growth of striped domains

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Abstract

We analyze the dynamical scaling behavior in a two-dimensional spin model with competing interactions after a quench to a striped phase. We measure the growth exponents studying the scaling of the interfaces and the scaling of the shrinking time of a ball of one phase plunged into the sea of another phase. Our results confirm the predictions found in previous papers. The correlation functions measured in the direction parallel and transversal to the stripes are different as suggested by the existence of different interface energies between the ground states of the model. Our simulations show anisotropic features for the correlations both in the case of single-spin-flip and spin-exchange dynamics.

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I. INTRODUCTION

When a system in a disordered phase is rapidly quenched to a temperature below its ordering temperature it orders kinetically [1,2]. In the early stage the fluctuations in the initial state are amplified and domains of macroscopic size are formed. At late time the ordering system is usually characterized by a single time-dependent length, the average domain size $R(t)$, which grows as a power law $R \sim t^\gamma$ (scaling regime) [3]. The growth exponent depends on the mechanism driving the phase separation. For a system with a scalar not-conserved order parameter (model A) the growth is curvature driven and $\gamma = \frac{1}{2}$ [4]. The mechanism in systems with conserved order parameter (model B) is the diffusion of the order parameter from interfaces of high curvature to regions of low curvature and $\gamma = \frac{1}{3}$ [5,6].

This work concerns the ordering in the Ising version of the bidimensional isotropic eight vertex model after a quench to the striped phase. The reduced hamiltonian of the model is

$$-\beta H = J_1 \sum_{\langle ij \rangle} s_i s_j + J_2 \sum_{\langle\langle ij \rangle\rangle} s_i s_j + J_3 \sum_{[i,j,k,l]} s_i s_j s_k s_l, \quad (1)$$

where s_i are Ising spins on a bidimensional square lattice and the sums are respectively on nearest neighbor pairs of spins, next to the nearest neighbor pairs and plaquettes. We have considered the case of periodic boundary conditions.

The quenching of model (1) to the ferromagnetic phase with $J_3 = 0$ has been studied in both two and three dimensions [7]. When $J_2 < 0$ there are energy barriers for the coarsening of domains, hence the system does not relax to equilibrium if the temperature is zero. These energy barriers do not increase with the linear dimension of domains in $D = 2$, while in $D = 3$ the energy barrier is proportional to the linear dimension of domains thus leading to a very slow dynamics [7].

The phase diagram of model (1) when $J_2 < 0$, $|J_1| < 2|J_2|$ and for J_3 small is characterized by a critical curve separating the paramagnetic phase and the superantiferromagnetic phases (see e. g. [8]). In the SAF case the model has four ground states consisting of alternate plus and minus rows (columns). The order parameter for SAF phases is the difference between the magnetization on odd and even rows (columns).

Quenching in the SAF phase, for model (1) in $D = 2$, has been studied in [9], where it has been shown that also in the striped phase the average size of domains grows as $R \sim t^\gamma$ where $\gamma = \frac{1}{2}$ or $\gamma = \frac{1}{3}$ for single-spin-flip or spin-exchange dynamics.

In a previous paper [10] we have shown that the correlation functions measured in the direction parallel and transversal to the stripes are different as suggested by the existence of different interface energies between the ground states of the model. Furthermore we furnished an explicit example of how the scaled correlation functions can depend on the details of the system (see also [11]). In this paper we complete the analysis described in [10].

In the next Section we concentrate on the scaling exponents and we confirm the values found in [9] by studying the scaling of the amount of interfaces and the scaling of the shrinking time of a “ball” of one phase plunged into a sea of a different phase.

In Section 3 we study the asymptotic correlations in the model. As to the single-spin-flip dynamics we show that the analysis of the pair correlation functions introduced in [9] gives

results indistinguishable from those obtained considering the longitudinal and transversal correlation functions as described in [10]. As to the spin-exchange dynamics we find an anisotropic behavior of the scaled correlation functions as well.

Section 4 is devoted to the conclusions.

II. DIFFERENT WAYS TO MEASURE GROWTH EXPONENTS

The growth exponents of domains after a quenching in the SAF phase have been already measured in [9]; it is interesting to measure those exponents studying the scaling properties of physical quantities different from those considered in [9].

In order to describe the main features of domains we remark that the ground state of the hamiltonian (1) is four-fold degenerate, so the typical configuration of the system in the scaling regime consists of a patchwork of domains of four types (see Fig. 1a). In the following we refer to domains having magnetized rows as “horizontal” domains, we call “vertical” domains those with magnetized columns.

First of all we studied the amount of interfaces (see Fig. 1b) present in the system to monitor the domain growth towards the equilibrium, that is to estimate the dimension of the domains. Indeed in two dimensions the total length of interfaces per unit volume scales as the inverse of the average size of domains (see [12] where the scaling of interfaces is used to measure the growth exponent in the case of ferromagnetic Ising model).

The definition of interfaces between different domains is not straightforward in the case of the superantiferromagnetic phase. In order to detect if a given site belongs to a domain or to the interface, we compare the configuration of the system in a neighborhood of the site with two given patterns in the following way: let us consider a site of the lattice, we denote it by the pair (i, j) , where i and j are respectively the row and column index, and we denote by $s(i, j)$ the corresponding spin. We consider a positive integer number L , denote by $B(i, j)$ the $(2L + 1) \times (2L + 1)$ square block centered at site (i, j) and compute the two following quantities

$$\begin{aligned} d_h &= \sum_{k,l=-L}^L \left(1 - \delta \left(s(i+k, j+l), (-1)^k s(i, j) \right) \right) \\ d_v &= \sum_{k,l=-L}^L \left(1 - \delta \left(s(i+k, j+l), (-1)^l s(i, j) \right) \right) \end{aligned} \tag{2}$$

where $\delta(\cdot, \cdot)$ is Kroneker’s delta. We remark that d_h and d_v provides, respectively, the “distance” in $B(i, j)$ between the present configuration and a SAF horizontal or vertical domain. If d_h or d_v are less than a fixed integer number M , we say that the site (i, j) belongs, respectively, to an horizontal or vertical SAF domain; otherwise we say that the site (i, j) is an interface site. All the results that will be described in this paper have been obtained with $L = 1$ and $M = 2$; we have checked that our results do not depend on the choice of the parameters L and M .

In Fig. 2 it is depicted the logarithm of the total number A of interface sites for a 512×512 lattice system as a function of the logarithm of the time in the case of finite temperature ($\beta = 1$) and parameters $J_1 = 0.1$, $J_2 = -1$ and $J_3 = 0.1$. Black circles and

black squares (above and below in the picture) are Monte Carlo results obtained averaging over 50 different histories respectively in the case of single-spin-flip [13] and spin-exchange dynamics [14]. We find the scaling law $A \sim t^{-\gamma}$ with $\gamma = \frac{1}{2}$ and $\gamma = \frac{1}{3}$ respectively in the case of single-spin-flip and spin-exchange dynamics, thus confirming the growth exponent found in [9].

The scaling law and the values of the exponent γ have been shown not to depend on the J 's and on the value of β . In the case of single-spin-flip dynamics the case of zero temperature [15] ($\beta = \infty$) has been considered, as well. We also checked that these results are not affected by finite size effects.

Another way of measuring the exponent γ , in the case of not-conserved dynamics, consists in studying the shrinking of a $L \times L$ square domain (ball) of one phase plunged into the sea of one of the three other phases. In Fig. 3 it is shown the shrinking of a 41×41 square vertical domain plunged into the sea of the horizontal superantiferromagnetic phase. The contraction of the ball is achieved via the corner erosion, indeed in this way no energy barrier must be bypassed. In [1] it has been remarked that the shrinking time τ of such a domain scales as $\tau \sim L^{\frac{1}{\gamma}}$. We found that the time of shrinking scales as $\tau \sim L^2$, see Fig. 4, for large L and for any choice of the phase of the background, this confirms the growth exponent $\gamma = \frac{1}{2}$.

III. ANISOTROPIC BEHAVIOR OF CORRELATION FUNCTIONS

Let us now turn to consider the correlation properties of growing domains in the scaling regime. In [10] we introduced two different types of correlation functions, the *longitudinal* and the *transverse* one; these two functions are denoted respectively by $C_\ell(r)$ and $C_t(r)$ and they are defined as follows

$$C_\ell(r, t) = \langle s(i, j) s(i + \epsilon(i, j)r, j + (1 - \epsilon(i, j))r) \rangle \quad (3)$$

$$C_t(r, t) = \langle (-1)^r s(i, j) s(i + (1 - \epsilon(i, j))r, j + \epsilon(i, j)r) \rangle$$

where $\epsilon(i, j)$ is one (zero) if site (i, j) belongs to a horizontal (vertical) domain and the average is performed over sites belonging to domains at time t (interface sites are excluded) and over different stories of the system. We remark that the longitudinal correlation function measures the correlation properties of domains in the direction where spins are aligned, while the transverse correlation function measures the correlation properties in the direction where the spins are alternate.

We found that the correlation functions introduced above have a scaling behavior in the scaling regime; in the case of single-spin-flip dynamics they depend only on the combination r/\sqrt{t} :

$$C_\ell(r, t) = f_\ell\left(\frac{r}{\sqrt{t}}\right) \quad C_t(r, t) = f_t\left(\frac{r}{\sqrt{t}}\right) \quad (4)$$

Simulations discussed in [10] have shown that the scaling functions f_ℓ and f_t are different, due to the presence of interfaces between the four types of domains having different interface

energies. The OJK theory [16] well describes the pair scaling functions in anisotropic cases if a free parameter is used to fit the data in the different directions (see [10]).

We also note that in this case two typical lengths characterize the ordering system, the average longitudinal domain size R_ℓ and the transverse one R_t ; we evaluated them as

$$R_\ell^{-1} = \frac{\sum k S_\ell(k)}{\sum S_\ell(k)} \quad R_t^{-1} = \frac{\sum k S_t(k)}{\sum S_t(k)} \quad (5)$$

where $S_\ell(k)$ and $S_t(k)$ are the Fourier transforms of $C_\ell(r)$ and $C_t(r)$ respectively. We verified that R_ℓ and R_t are different but they both have the correct scaling $R_\ell \sim t^{\frac{1}{2}}$ and $R_t \sim t^{\frac{1}{2}}$.

Now we check that the anisotropic behavior of domains growth does not depend on the peculiar way in which (3) measure the correlations, indeed we show that the analysis of the pair correlation functions introduced in [9] yields similar results.

As in [9] let us divide the lattice into four sublattices corresponding to a 2×2 unit cell; a two-components order parameter $\Psi = \{\psi_a\}_{a=1,2}$ can be expressed in terms of the sublattices magnetizations m_1, m_2, m_3 and m_4 , where $m_\nu = \frac{1}{N} \sum_{i \in \nu} s_i$ and N is the total number of sites in the lattice, by defining

$$\psi_1 = m_1 + m_2 - m_3 - m_4 \quad \psi_2 = m_1 - m_2 - m_3 + m_4 \quad . \quad (6)$$

The four ground states of model (1) correspond to the four following values of the order parameter Ψ :

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \begin{pmatrix} -1 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \begin{pmatrix} 0 \\ -1 \end{pmatrix} \quad . \quad (7)$$

We observe that $|\psi_1| = 1$ ($|\psi_2| = 1$) corresponds to a striped phase in the direction parallel to the x (y) axis.

By decomposing Ψ into its contributions from individual unit cells Ψ_α , where α is the cell index, one can consider the correlation between the components of the two-valued order parameter. Two of such correlations can be put in correspondence with the longitudinal and transverse correlation functions (3). Indeed, let us consider two cells α and α' connected by a vector parallel to the x axis: it is easy to see that the average of the product $\psi_{\alpha,1}\psi_{\alpha',1}$ measures the longitudinal correlations, while the averaged $\psi_{\alpha,2}\psi_{\alpha',2}$ is a measure of the transverse correlations in the growing system. Conversely, given two cells connected by a vector parallel to the y axis, $\psi_{\alpha,1}\psi_{\alpha',1}$ and $\psi_{\alpha,2}\psi_{\alpha',2}$ measure respectively the transverse and the longitudinal correlations. In this framework the natural way to define transverse and longitudinal correlation functions is the following:

$$\begin{aligned} \Gamma_\ell(r, t) &= \frac{1}{2} \langle \psi_{\alpha,1} \psi_{\alpha+r\vec{x},1} \rangle + \frac{1}{2} \langle \psi_{\alpha,2} \psi_{\alpha+r\vec{y},2} \rangle \\ \Gamma_t(r, t) &= \frac{1}{2} \langle \psi_{\alpha,1} \psi_{\alpha+r\vec{y},1} \rangle + \frac{1}{2} \langle \psi_{\alpha,2} \psi_{\alpha+r\vec{x},2} \rangle \end{aligned} \quad (8)$$

where \vec{x} and \vec{y} are the unit vectors in the x and y directions and the average is performed over all the cells at time t and over different stories of the system.

Although C 's and Γ 's are defined in a slightly different way, we note that from the physical point of view they are expected to satisfy the following identities

$$\Gamma_\ell(r, t) = C_\ell(2r, t) \quad \Gamma_t(r, t) = C_t(2r, t) \quad , \quad (9)$$

where the factor 2 in the argument of the C 's is due to the fact that the dynamical variables Ψ_α live on a lattice with spacing which is twice the original one.

In Fig. 5 we show the scaling collapse of the correlation functions Γ_ℓ and Γ_t . Data in Fig. 5 above (below) have been obtained by Monte Carlo simulations performed on a 400×400 lattice system with a single-spin-flip dynamics, at zero temperature and parameters $J_1 = 0.1$ ($J_1 = -0.1$), $J_2 = -1$ and $J_3 = 0$. The correlation functions (8), taken at different times, have been plotted in terms of the scaling variable $z = r/\sqrt{t}$. From the picture it is clear that the anisotropy is confirmed and that a symmetric behavior with respect to the change of the sign of J_1 is observed.

Solid lines in Fig. 5 represent the best fit of our data obtained with the OJK function

$$f(z) = \frac{2}{\pi} \sin^{-1}[\exp(-z^2/D)] \quad ; \quad (10)$$

the optimal choices of the parameter D is $D_\ell = 1.35$ (1.15) and $D_t = 1.15$ (1.35) respectively for the longitudinal and transverse function in the case $J_1 = 0.1$ (-0.1). The validity of the identities (9) is confirmed by the fact that the best fits of the D 's, in the case of the C 's (see [10]), are close to be four times the best fits of the D 's in the case of the Γ 's functions.

Finally we discuss the simulations we have performed with spin-exchange dynamics. We used heat bath spin-exchange between nearest neighbor pairs of spins [14]. In Fig. 6 the collapse of correlation functions (3) is shown: Monte Carlo data have been plotted in terms of the scaling variable $z = r/t^{1/3}$. Simulations have been performed on a 800×800 lattice, at inverse temperature $\beta = 1$ and parameters $J_1 = 0.4$, $J_2 = -1$ and $J_3 = 0$. We see that the anisotropic behavior is observed in the case of the spin-exchange dynamics as well. Again we found that the longitudinal and the transverse correlation functions are exchanged when $J_1 \rightarrow -J_1$.

IV. CONCLUSIONS

In this paper we have further analyzed the dynamical scaling behavior in a two-dimensional spin model with competing interactions which had been already investigated in [9,10]. We measured the growth exponents studying physical magnitudes not considered in previous papers: the scaling of the interfaces and the scaling of the shrinking time of a ball of one phase plunged in the sea of another phase. Our results confirm the predictions found in [9,10].

The anisotropic behavior of the correlations has been further investigated by measuring the pair correlation functions introduced in [9] and their physical equivalence with the correlation functions used in [10] has been pointed out. Our simulations show anisotropic features for the correlations in growing system and the symmetric behavior with respect to the change of the sign of the nearest neighbors coupling. Finally, we have shown that the anisotropy is observed also in the case of spin exchange dynamics.

REFERENCES

- ¹ A.J. Bray, Adv. Phys. **43**, 357 (1994).
- ² J.D. Gunton et al., in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, New York, 1983), Vol.8.
- ³ S.F. Bates, Science **251**, 898 (1991).
- ⁴ I.M. Lifshitz, Zh. Eksp. Teor. Fiz. **42**, 1354 (1962); S.M. Allen, J.W. Cahn, Acta. Metall. **27**, 1085 (1979).
- ⁵ I.M. Lifshitz, V.V. Slyozov, J. Chem. Solids **19**, 35 (1961).
- ⁶ M. Rao, M.H. Kalos, J.L. Lebowitz, J. Marro, Phys. Rev. B **13**, 4328 (1976); J.F. Marko, J.T. Barkema, Phys. Rev. E **52**, 2522 (1995).
- ⁷ J.D. Shore, M. Holzer, J.P. Sethna, Phys. Rev. B **46**, 11379 (1992); M. Rao, A. Chakrabarti, Phys. Rev. E **52**, R13 (1995).
- ⁸ R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982).
- ⁹ A. Sadiq, K. Binder, Journ. Stat. Phys. **35**, 517 (1984).
- ¹⁰ E.N.M. Cirillo, G. Gonnella, S. Stramaglia, in press on Phys. Rev. E.
- ¹¹ A.D. Rutenberg, Phys. Rev. E **54**, R2181 (1996).
- ¹² K. Humayun, A. Bray, J. Phys. A: Math. Gen. **24**, 1915 (1991).
- ¹³ R.J. Glauber, Jour. Math. Phys. **4**, 294 (1962).
- ¹⁴ K. Kawasaki, in *Phase Transitions and Critical Phenomena*, Vol.2, edited by C. Domb and M. Green (Academic Press, London, 1970).
- ¹⁵ The spin is flipped with probability 1 if $\Delta H < 0$, with probability 0.5 if ΔH vanishes and is not flipped if ΔH is positive; ΔH is the variation of the hamiltonian corresponding to the spin flip.
- ¹⁶ T. Ohta, D. Jasnow, K. Kawasaki, Phys. Rev. Lett. **49**, 1223 (1982).

Figure Captions

Fig 1: (a) Typical configuration of model (1) in the scaling regime. Black (white) squares represent plus (minus) spins. The picture has been obtained in a 100×100 square lattice, at zero temperature, after 150 MCS (Monte Carlo Steps per site). (b) The same configuration as in Fig. 1a is depicted. Black squares represent the interface sites and grey (white) squares represent plus (minus) spins belonging to domains (see the definitions in the text).

Fig 2: The logarithm of the number A of interface sites is plotted versus the logarithm of the time t (number of iterations) in a 512×512 square lattice. Black circles (above) and black squares (below) are Monte Carlo results obtained averaging over 50 different histories respectively in the case of single-spin-flip and spin-exchange dynamics. In both cases the inverse temperature is $\beta = 1$ and the parameters of the model have been chosen as follows: $J_1 = 0.1$, $J_2 = -1$ and $J_3 = 0.1$. The slope of the solid line is $-\frac{1}{2}$ above and $-\frac{1}{3}$ below.

Fig. 3: The shrinking of a 41×41 vertical domain plunged into the horizontal SAF phase is shown. Our simulation has been performed on a 100×100 square lattice, at zero temperature and with parameters $J_1 = 0.1$, $J_2 = -1$ and $J_3 = 0$. Black (white) squares represent plus (minus) spins; from the left to the right and from the top to the bottom configurations are shown at times $t = 0, 50, 100, 150, 200, 225$.

Fig 4: The logarithm of the collapse time τ of a square vertical domain plunged into the horizontal SAF phase is plotted versus the logarithm of the length L of its side. Black squares are Monte Carlo data obtained by averaging over 10 different trials in the zero temperature case with parameters $J_1 = 0.1$, $J_2 = -1$ and $J_3 = 0$. The slope of the solid line is 2. Similar results have been obtained when different background phases were considered.

Fig 5: Scaling collapse of the correlation functions $\Gamma_\ell(r, t)$ and $\Gamma_t(r, t)$ achieved by plotting them versus $r/t^{0.5}$. Results are given for $\beta = \infty$, $J_2 = -1$, $J_3 = 0$, $J_1 = 0.1$ above and $J_1 = -0.1$ below; we averaged over 50 different histories on a 400×400 system. Black (empty) circles, squares and triangles correspond respectively to the transverse (longitudinal) correlation functions measured at times 300, 400 and 500. Solid lines are the best OJK fits.

Fig 6: Scaling collapse of the correlation functions $C_\ell(r, t)$ and $C_t(r, t)$ achieved by plotting them versus the scaling variable $r/t^{1/3}$. Results are given for $\beta = 1$, $J_1 = 0.4$, $J_2 = -1$ and $J_3 = 0$; we averaged Monte Carlo data over 50 different stories on a 800×800 system. Both the longitudinal and transverse correlation functions are shown at times 68000 (\circ), 70000 (\square) and 72000 (\triangle).

FIGURES

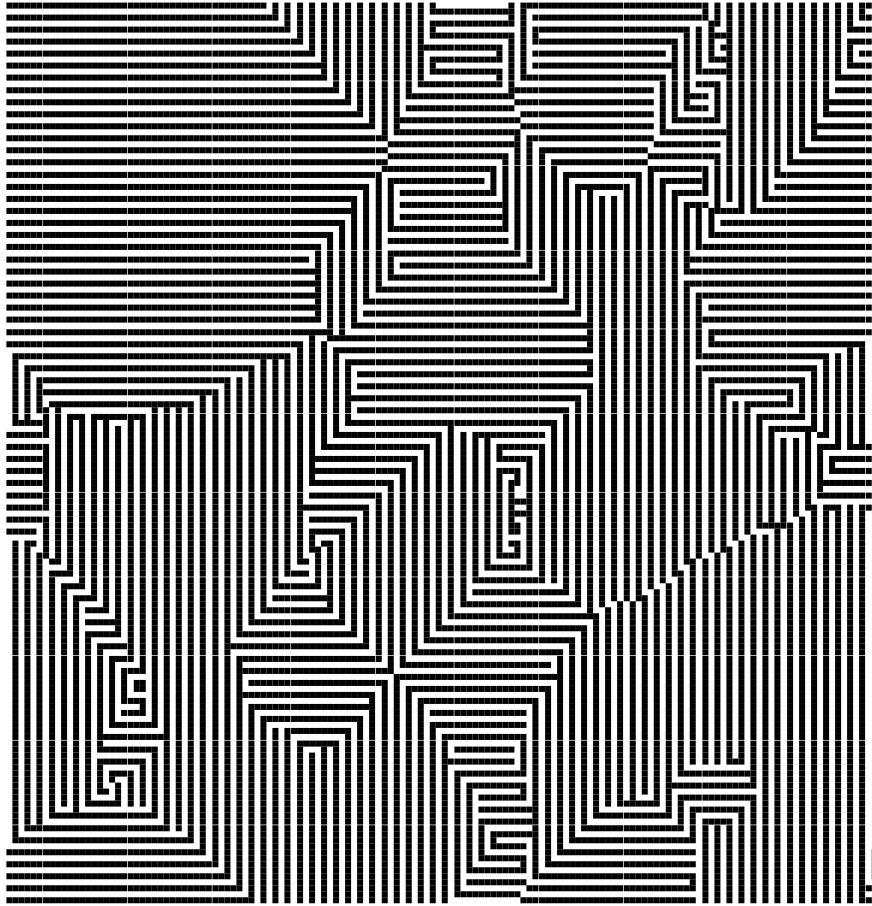


Fig. 1a - Cirillo, Gonnella, Stramaglia

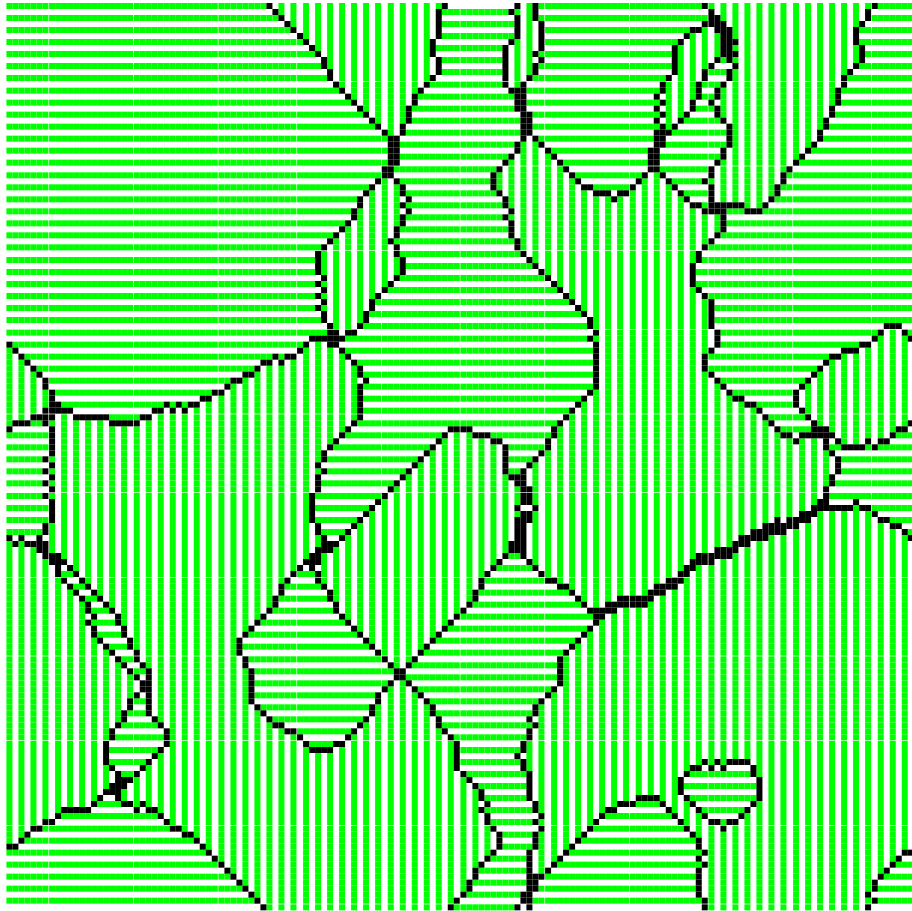


Fig. 1b - Cirillo, Gonnella, Stramaglia

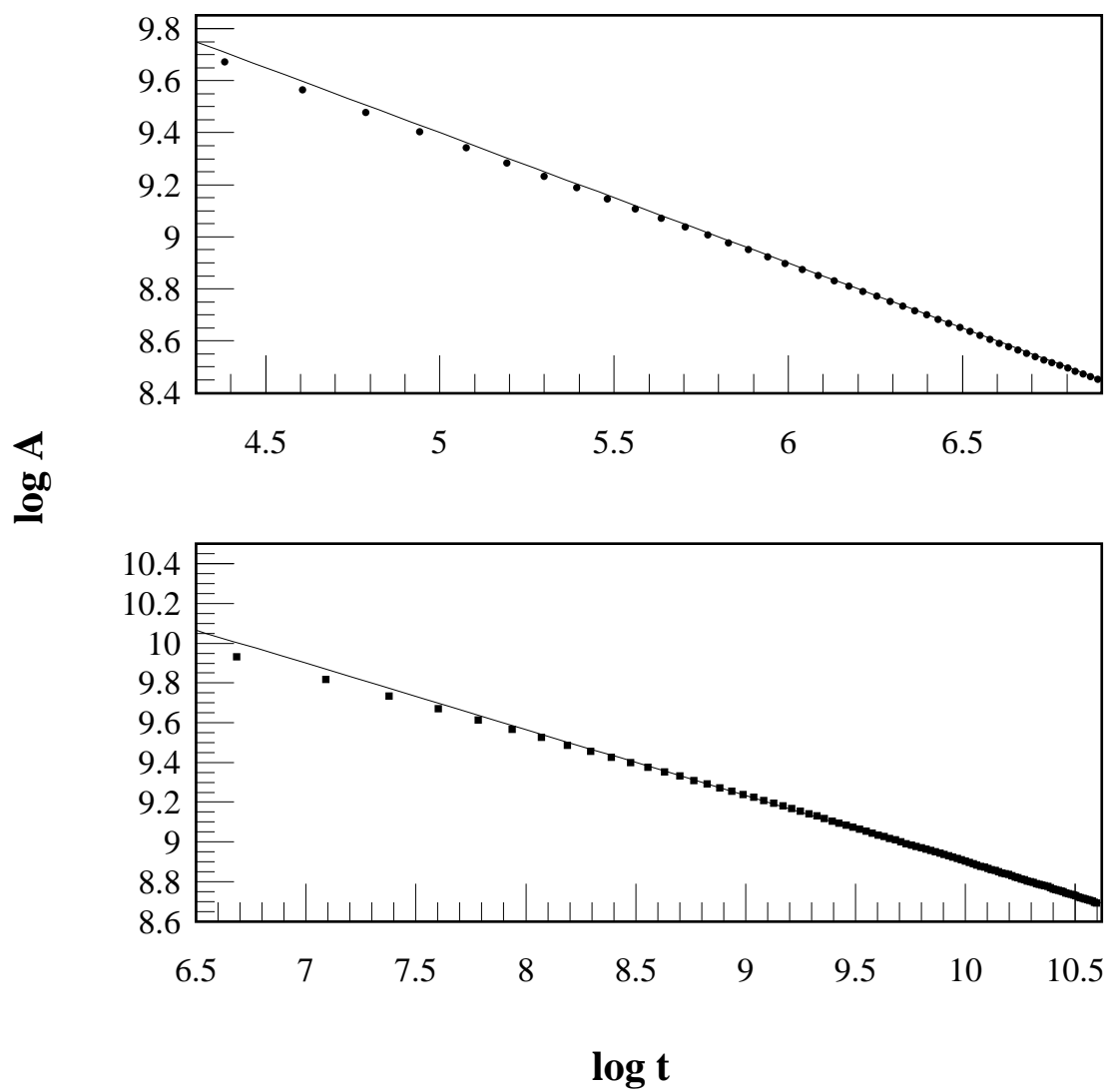


Fig. 2 - Cirillo, Gonnella, Stramaglia

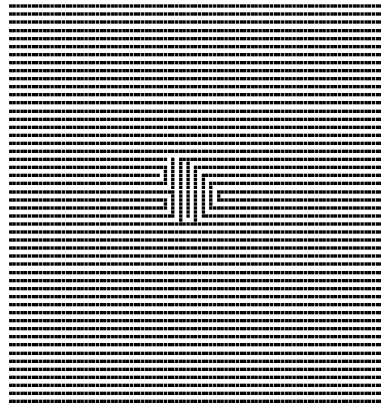
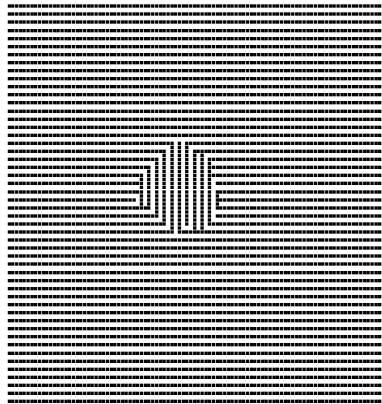
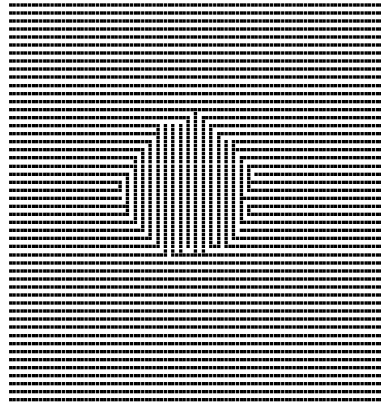
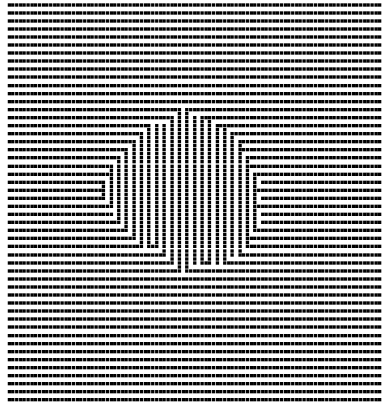
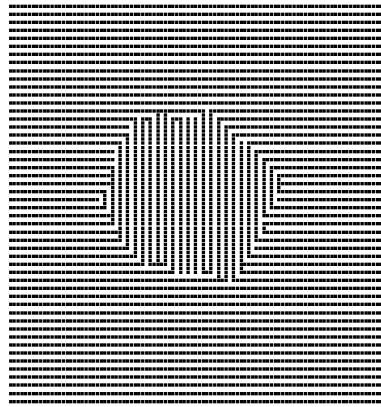
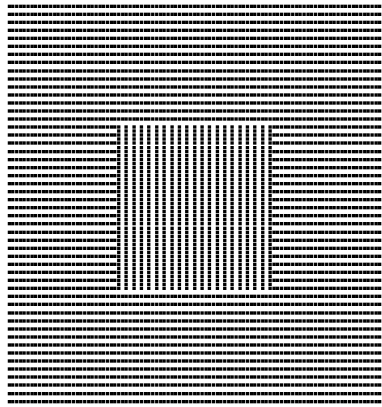


Fig. 3 - Cirillo, Gonnella, Stramaglia

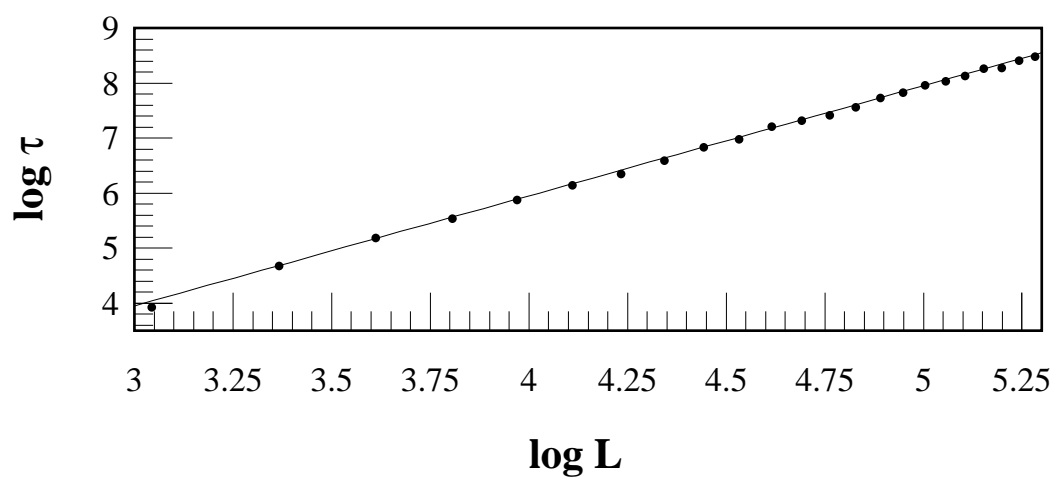


Fig. 4 - Cirillo, Gonnella, Stramaglia

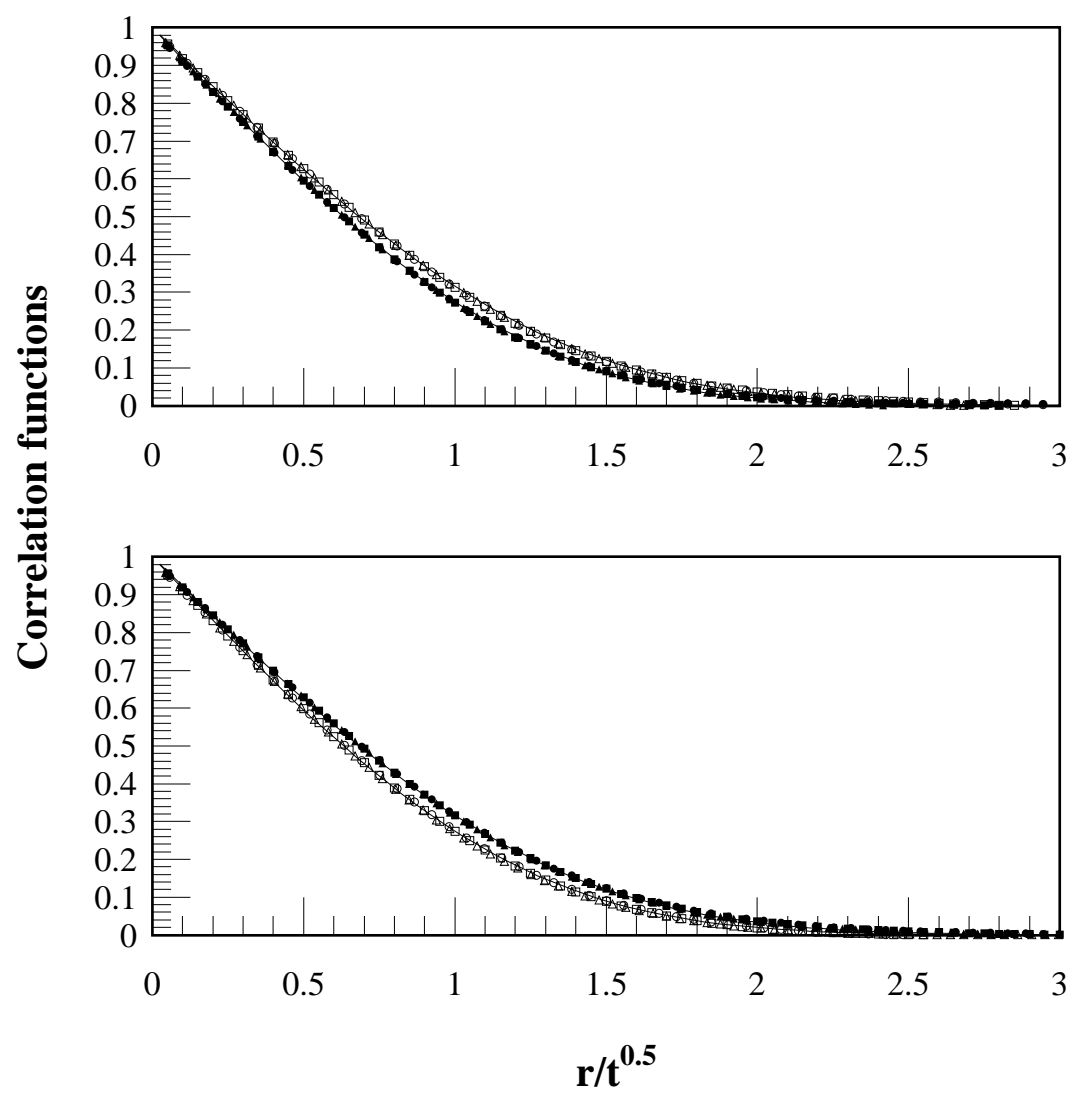


Fig. 5 - Cirillo, Gonnella, Stramaglia

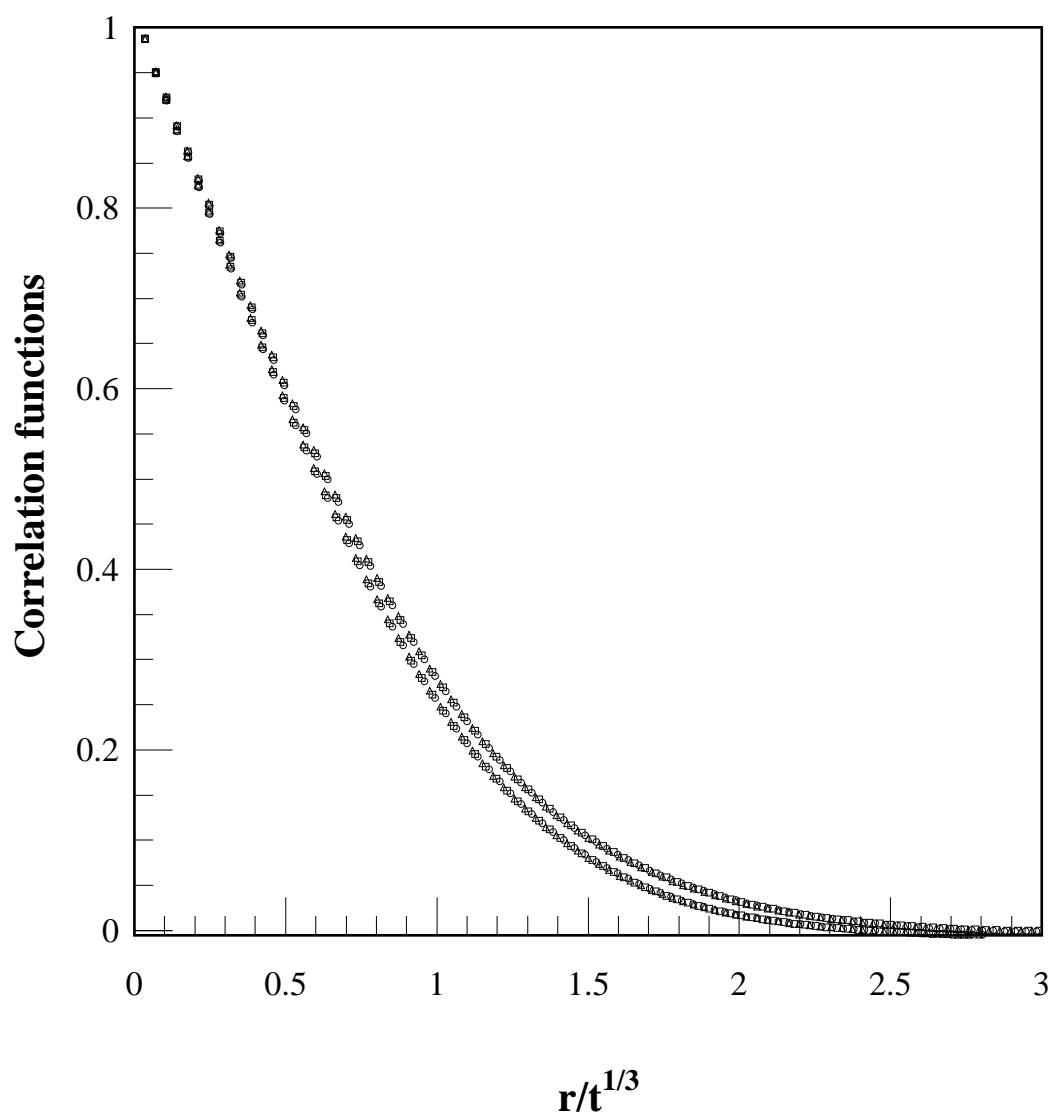


Fig. 6 - Cirillo, Gonnella, Stramaglia